

Supporting Information

**Silicon Nanowires Decorated with Gold Nanoparticles via *In-Situ* Reduction for
Photoacoustic Imaging-guided Photothermal Cancer Therapy**

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1. Calculation of the photothermal conversion efficiency

Following Roper's report, the total energy balance for the system can be expressed by

Eq. 1:

$$\sum_i m_i C_{p,i} \frac{dT}{dt} = Q_{NC} + Q_{Dis} - Q_{Surr} \quad (1),$$

where m and C_p are the mass and heat capacity of water, respectively, T is the solution temperature, Q_{NC} is the energy inputted by NCs, Q_{Dis} is the baseline energy inputted by the sample cell, and Q_{Surr} is heat conduction away from the system surface by air.

The laser-induced source term, represents heat dissipated by electron-phonon relaxation of the plasmons on SiNWs-AuNPs surface under the irradiation of 1064 nm laser:

$$Q_{NC} = I(1 - 10^{-A_{1064}})\eta \quad (2),$$

where I is incident laser power, η is the conversion efficiency from incident laser energy to thermal energy, and A_{1064} is the absorbance of the SiNWs-AuNPs at wavelength of 1064 nm. In addition, source term, Q_{Dis} , expresses heat dissipated from light absorbed by the quartz sample cell itself, and it was measured independently to be 10.9 mW using a quartz cuvette cell containing pure water without a SiNWs-AuNPs. Furthermore, Q_{Surr} is linear with temperature for the outgoing thermal energy, as given by Eq. 3:

$$Q_{Surr} = hs(T - T_{Surr}) \quad (3),$$

where h is heat transfer coefficient, s is the surface area of the container, and T_{Surr} is ambient temperature of the surroundings.

Once the laser power is defined, the heat input ($Q_{\text{NC}} + Q_{\text{Dis}}$) will be finite. Since the heat output (Q_{Surr}) is increased along with the increase of the temperature according to the Eq. 3, the system temperature will rise to a maximum when the heat input is equal to heat output:

$$Q_{\text{NC}} + Q_{\text{Dis}} = Q_{\text{Surr-Max}} = hs(T_{\text{Max}} - T_{\text{Surr}}) \quad (4),$$

where the $Q_{\text{Surr-Max}}$ is heat conduction away from the system surface by air when the sample cell reaches the equilibrium temperature, and T_{max} is the equilibrium temperature. The 1064 nm laser heat conversion efficiency (η) can be determined by substituting Eq. 2 for Q_{NC} into Eq. 4 and rearranging to get

$$\eta = \frac{hs(T_{\text{Max}} - T_{\text{Surr}}) - Q_{\text{Dis}}}{I(1 - 10^{-A_{1064}})} \quad (5),$$

where Q_{Dis} was measured independently to be 10.9 mW, the $(T_{\text{max}} - T_{\text{Surr}})$ was 21.6 °C according to Figure 3g, I is 1.0 mW/cm², A_{1064} is the absorbance (0.46949) of SiNWs-AuNPs at 1064 nm (Figure S3a). Thus, only the hs remains unknown for calculating η . In order to get the hs , a dimensionless driving force temperature, θ is introduced using the maximum system temperature, T_{max}

$$\theta = \frac{T - T_{\text{Surr}}}{T_{\text{Max}} - T_{\text{Surr}}} \quad (6),$$

and a sample system time constant τ_s

$$\tau_s = \frac{\sum_i m_i C_{p,i}}{hs} \quad (7),$$

which is substituted into Eq. 1 and rearranged to yield

$$\frac{d\theta}{dt} = \frac{1}{\tau_s} \left[\frac{Q_{NC} + Q_{Dis}}{hs(T_{Max} - T_{Surr})} - \theta \right] \quad (8),$$

At the cooling stage of the aqueous dispersion of the SiNWs-AuNPs, the light source was shut off, the $Q_{NC} + Q_{Dis} = 0$, reducing the Eq. 9

$$dt = -\tau_s \frac{d\theta}{\theta} \quad (9),$$

and integrating, giving the expression

$$t = -\tau_s \ln\theta \quad (10),$$

Therefore, time constant for heat transfer from the system is determined to be $\tau_s = 265.8$ s by applying the linear time data from the cooling period (after 600 s) vs negative natural logarithm of driving force temperature (Figure 3h). In addition, the m is 0.5 g and the C is 4.2 J/g. Thus, according to Eq. 7, the hs is deduced to be 7.7 mW/°C. Substituting 7.7 mW/°C of the hs into Eq. 5, the 1064 nm laser heat conversion efficiency (η) of SiNWs-AuNPs can be calculated to be 24.1%. The calculation method of the photothermal conversion efficiency of pure SiNWs suspensions was similar to the one of SiNWs-AuNPs and the efficiency of pure SiNWs was 12.2% (Figure S4).

2. Supporting Figures

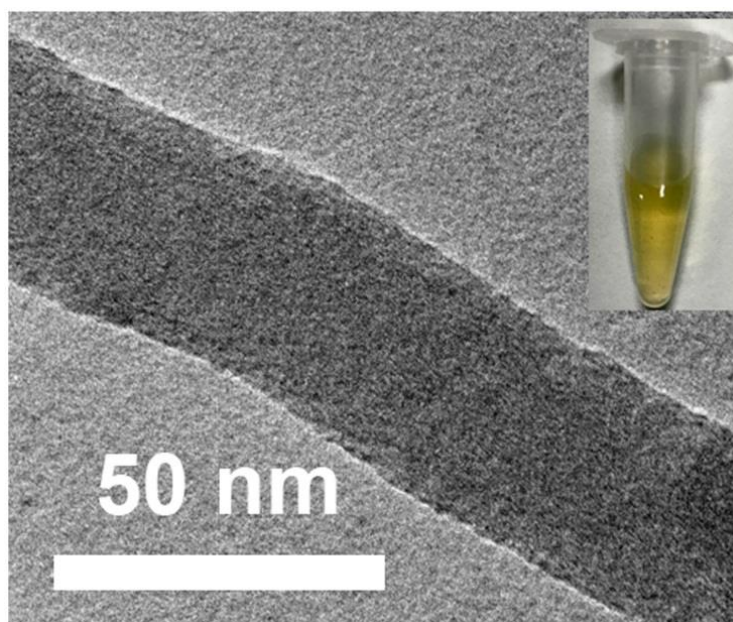


Figure S1. TEM image of a pristine SiNW, the insert image being the appearance of SiNW dispersion.

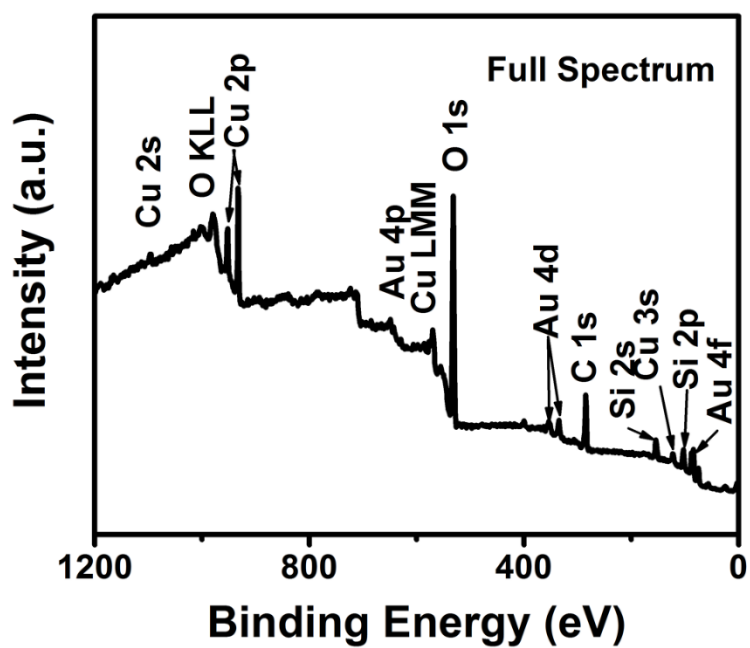


Figure S2. XPS full spectrum of SiNWs-AuNPs (copper sheets as substrates).

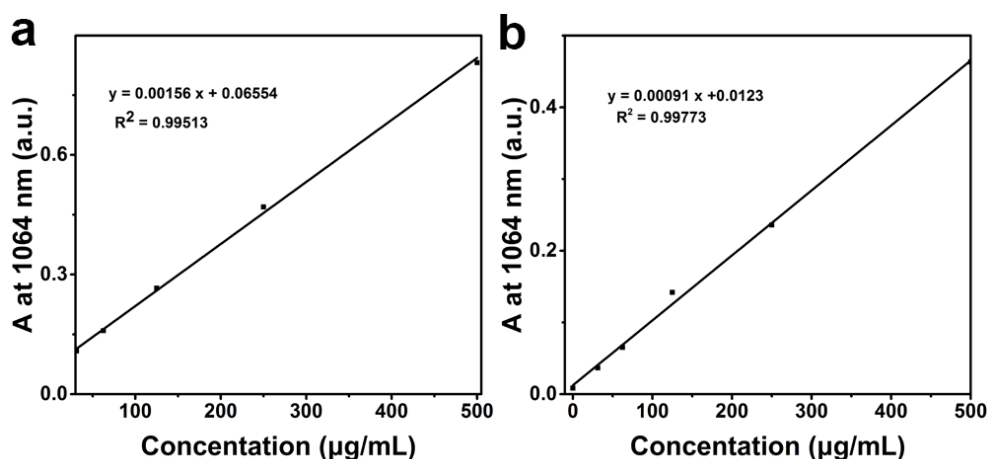


Figure S3. Normalized absorbance intensity with different concentrations at 1064 nm of (a) TA-SiNWs-AuNPs and (b) pure SiNWs suspensions (A means absorbance).

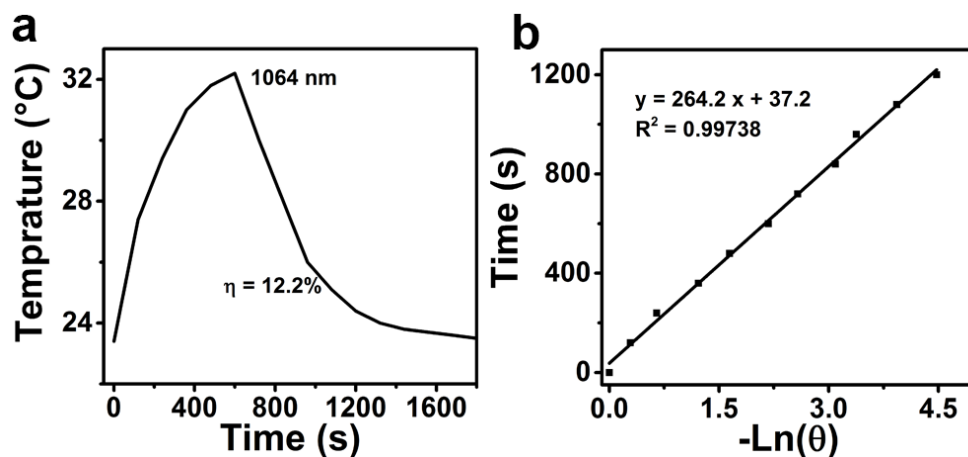


Figure S4. (a) Temperature profile of pure SiNWs suspensions (300 µg/mL) irradiated by 1064 nm laser (1.0 W/cm²) for 10 min followed by natural cooling with the laser turned off; and (b) Measuring the time constant for heat transfer from the system using a linear regression of cooling profile.

Table S1. Photothermal performance of reported PTAs in the NIR-II region

PTAs	Con ($\mu\text{g/mL}$)	Power (W/cm^2)	ΔT ($^{\circ}\text{C}$)	PTCE	Refs
Ultrathin PPy Nanosheets	100	1	40.2	64.6%	Nano Letters. 2018, 18, 2217
PEGylated Cu_3BiS_3 Nanorods	150	1	27	40.7%	Biomaterials. 2017, 112, 164.
Au@ Cu_{2-x}S Nanocrystals	200	0.7	20.5	43.3%	Adv. Mater. 2016, 28, 3094.
Au- Cu_9S_5 Nanoparticles	50	0.7	19.6	37%	J. Am. Chem. Soc. 2014, 136, 15684.
Fe_3O_4 @CuS-PEG Nanoparticles	300	3	22	19.2%	Adv. Funct. Mater. 2015, 25, 6527.
H- SiO_x -PEG Nanoparticles	36	1	23.5	48.6%	Biomaterials. 2017, 143, 120.
CoP-Nanocrystals	200	0.8	29.1	21.2%	Small. 2017, 13, 1700798.
Au Nanorod@PPy@ Fe_xO Nanocomposites	200	1	16.5	46.0%	Nano Research. 2016, 9, 787.
Fe_3O_4 Nanoclusters	375	0.38	24	20.8%	Nanoscale. 2015, 7, 12689.
$(\text{NH}_4)_x\text{WO}_3$ Nanocubes	250	1.4	24.8	39.4%	Biomaterials. 2015. 02. 054
SiNWs-AuNPs	300	1	21.6	24.1%	This work